

2,4,5-trichlorophenacylchloride

Inchi:	InChI=1S/C8H6Cl4/c9-2-1-5-3-7(11)8(12)4-6(5)10/h3-4H,1-2H2
InchiKey:	ICOVPLQFGDISSG-UHFFFAOYSA-N
Formula:	C8H6Cl4
SMILES:	ClCCc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	243.94

Physical Properties

Property code	Value	Unit	Source
gf	52.28	kJ/mol	Joback Method
hf	-69.29	kJ/mol	Joback Method
hfus	26.14	kJ/mol	Joback Method
hvap	55.20	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.428		Crippen Method
mcvol	148.780	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	573.78	K	Joback Method
tc	809.85	K	Joback Method
tf	363.58	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.35	J/molxK	573.78	Joback Method
cpg	278.20	J/molxK	613.13	Joback Method
cpg	286.46	J/molxK	652.47	Joback Method
cpg	294.14	J/molxK	691.82	Joback Method
cpg	301.28	J/molxK	731.16	Joback Method

cpg	307.89	J/mol×K	770.51	Joback Method
cpg	314.02	J/mol×K	809.85	Joback Method
dvisc	0.0013128	Paxs	363.58	Joback Method
dvisc	0.0008856	Paxs	398.61	Joback Method
dvisc	0.0006366	Paxs	433.65	Joback Method
dvisc	0.0004808	Paxs	468.68	Joback Method
dvisc	0.0003776	Paxs	503.71	Joback Method
dvisc	0.0003060	Paxs	538.75	Joback Method
dvisc	0.0002544	Paxs	573.78	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R141583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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